Predicting thermoelastic properties of materials with advanced exchange correlation functionals

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Idioma Sin definir

Descripción:
Proyecto asignado a través de la Red Española de Supercomputación [2].

Thermoelastic properties of materials are essential to understand the behavior of Earth-forming minerals at high pressures and temperatures or the use of ultra-high temperature ceramics at aerospace applications. However, the computational prediction of the properties is extremely expensive. We have developed a methodology to finite temperature properties such as elastic constants and other mechanical properties such as bulk modulus, shear modulus, Poisson ratio, Young modulus or elastic anisotropy, reducing the computational cost of traditional approaches. However, many questions related to the performance of different exchange correlation functions to predict these properties remains unsolved. In this activity, we strive to calculate thermoelastic properties of a benchmark of materials using different functionals.

Web:

URL del envío:https://www.cenits.es/proyectos/predicting-thermoelastic-properties-materials-advanced-exchange-correlation-functionals

Enlaces
[1] http://www.us.es/ [2] https://www.res.es/